

=> d his

(FILE 'HOME' ENTERED AT 10:12:38 ON 17 JUN 2003)

FILE 'CA' ENTERED AT 10:12:50 ON 17 JUN 2003

L1 15580 S (MASS OR SPECIE) (2A) (BALANCE OR CONVER? OR INTERCONVER?)
L2 24567 S CRIII OR CRVI OR (CR OR CHROMIUM) (W) (III OR VI)
L3 34 S L1 AND L2
L4 1231 S L1 AND (ISOTOP? OR SPIKE OR (STANDARD OR LABEL?) (2A) (ADDITION OR ADD
OR ADDING OR ENRICH?))
L5 112 S L4 AND MASS SPEC?
L6 472 S L4 AND (ION? OR ANION? OR CATION? OR TRACE OR REDOX OR REDUC? OR
OXID?)
L7 12 S L6 AND SPECIAT?
L8 300 S L4 AND REACT?
L9 12 S L7 AND SPECIAT?
L10 118 S L5, L7, L9
L11 17 S L10 AND ISOTOP? (1A) DILUT?
L12 77 S L10 NOT PY>1997
L13 2 S L10 NOT L12 AND PATENT/DT
L14 83 S L11-13

=> d bib, ab 1-83 114

L14 ANSWER 4 OF 83 CA COPYRIGHT 2003 ACS
AN 129:144450 CA
TI [Human] **Mass balance**/metabolite identification
AU Browne, Thomas R.; Szabo, George K.; Ajami, Alfred
CS Departments of Neurology and Pharmacology, Boston University School of
Medicine, USA
SO Pharmacochemistry Library (1997), 26 (Stable Isotopes in Pharmaceutical
Research), 219-232
AB A review, with 12 refs., on general methods for performing a **mass
balance**/metabolite identification study on any new drug using stable
isotope labeling and detection as an alternative to radioactive labeling
and detection. Continuous flow-**isotope** ratio **mass spectrometry** and chem.
reaction interface **mass spectrometry** are discussed.

L14 ANSWER 8 OF 83 CA COPYRIGHT 2003 ACS
AN 128:105811 CA
TI Low-temperature pyrolysis of CCA-treated wood waste: chemical determination
and statistical analysis of metal input and output; **mass balances**
AU Helsen, L.; Van Den Bulck, E.; Van Den Broeck, K.; Vandecasteele, C.
CS Department of Mechanical Engineering, Katholieke Universiteit Leuven,
Heverlee, 3001, Belg.
SO Waste Management (Oxford) (1997), 17(1), 79-86
AB Low-temp. pyrolysis is proposed as an alternative method to dispose of CCA-
treated wood waste. In the frame of a study aiming at optimizing the
pyrolysis of CCA-treated wood, an exptl. facility has been built to examine
the influence of important process parameters (pyrolysis temp., residence
time, heating rate, particle size,) on the release of metals and on the
resultant mass redn. In order to perform a **mass balance** calcn. for the
total system, a method for metal anal. was developed. Two leaching
procedures and one dissoln. procedure were tested and compared with each
other, resulting in an optimal procedure to bring the metals into soln.:
"the BSI method" to det. the total amt. of Cr, Cu and As in the dried wood
and "the Reflux method" to det. the total amt. of Cr, Cu and As in the
pyrolysis residue. These results illustrate that Cr is more strongly bound
in the pyrolysis residue as compared to the CCA-treated wood. The anal.

technique used was inductively coupled plasma-mass spectrometry, and the anal. problems like interferences and matrix effects were solved by using the appropriate **isotope**, an internal std., and math. corrections. The resulting optimal technique for CCA-treated wood ("the BSI method") was applied to wood samples with different particle sizes. A statistical anal. of the Cr, Cu, and As content in the CCA-treated wood shows the heterogeneous character of CCA-treated wood samples. Heterogeneity becomes less important when using samples with a small range of particle sizes. The smaller wood particles have significantly higher metal concns. than the larger particles. Realistic **mass balances** for the metals were obtained and showed that most of the Cr, Cu, and As remained in the pyrolysis residue.

L14 ANSWER 16 OF 83 CA COPYRIGHT 2003 ACS

AN 124:93073 CA

TI Gas Chromatographic Isolation of Individual Compounds from Complex Matrixes for Radiocarbon Dating

AU Eglinton, Timothy I.; Aluwihare, Lihini I.; Bauer, James E.; Druffel, Ellen R. M.; McNichol, Ann P.

CS Department of Marine Chemistry and Geochemistry, Woods Hole Oceanographic Institution, Woods Hole, MA, 02543, USA

SO Analytical Chemistry (1996), 68(5), 904-12

AB This paper describes the application of a novel, practical approach for isolation of individual compds. from complex org. matrixes for natural abundance radiocarbon measurement. This is achieved through the use of automated preparative capillary gas chromatog. (PCGC) to sep. and recover sufficient quantities of individual target compds. for ^{14}C anal. by accelerator **mass spectrometry** (AMS). This approach was developed and tested using a suite of samples (plant lipids, petroleums) whose ages spanned the ^{14}C time scale and which contained a variety of compd. types (fatty acids, sterols, hydrocarbons). Comparison of individual compds. and bulk radiocarbon signatures for the **isotopically** homogeneous samples studied showed that $\Delta^{14}\text{C}$ values generally agreed well ($\pm 10\%$). Background contamination was assessed at each stage of the isolation procedure, and incomplete solvent removal prior to combustion was the only significant source of addnl. carbon. **Isotope** fractionation was addressed through compd.-specific stable carbon **isotopic** analyses. Fractionation of **isotopes** during isolation of individual compds. was minimal (< 5 permill. for $\delta^{13}\text{C}$), provided the entire peak was collected during PCGC. Trapping of partially co-eluting peaks did cause errors, and these results highlight the importance of conducting stable carbon **isotopic** measurements of each trapped compd. in concert with AMS for reliable radiocarbon measurements. The addn. of carbon accompanying derivatization of functionalized compds. (e.g., fatty acids and sterols) prior to chromatog. sepn. represents a further source of potential error. This contribution can be removed using a simple **isotopic mass balance** approach. Based on these preliminary results, the PCGC-based approach holds promise for accurately detg. ^{14}C ages on compds. specific to a given source within complex, heterogeneous samples.

L14 ANSWER 27 OF 83 CA COPYRIGHT 2003 ACS

AN 121:220675 CA

TI Derivatization of organic compounds prior to gas chromatographic-combustion-**isotope** ratio **mass spectrometric** analysis: identification of **isotope** fractionation processes

AU Rieley, Gareth

CS School of Chemistry, University of Bristol, Bristol, BS8 1TS, UK

SO Analyst (Cambridge, United Kingdom) (1994), 119(5), 915-19

AB An examn. of the practice of derivatizing org. compds. such as fatty acids, sterols and amino acids in relation to subsequent anal. via gas chromatog.-

combustion-isotope ratio mass spectrometry is presented. Fractionation processes, such as kinetic isotope effects, which cause a deviation in the measured stable C isotope ratios (δ -values) of derivatized compds. from simple mass balance considerations are examd. Particular attention is paid to reactions that proceed by the cleavage of a C-contg. bond and reactions that probably have kinetic isotope effects assocd. with them, such as acetylation and diazotization. Isotope fractionation processes other than those which are kinetic based are also discussed, as is the addnl. imprecision of the calcn. of the δ -values of sample compds. inherent when deriv. C is added. Failure to take this imprecision into account when comparing δ -values could lead to erroneous conclusions with respect to the magnitude of kinetic isotope effects caused by deriv. reactions.

L14 ANSWER 38 OF 83 CA COPYRIGHT 2003 ACS

AN 114:61125 CA

TI Stable carbon isotope analysis of amino acid enantiomers by conventional isotope ratio mass spectrometry and combined gas chromatography/isotope ratio mass spectrometry

AU Silfer, J. A.; Engel, M. H.; Macko, S. A.; Jumeau, E. J.

CS Sch. Geol. Geophys., Univ. Oklahoma, Norman, OK, 73019, USA

SO Analytical Chemistry (1991), 63(4), 370-4

AB The application of a combined gas chromatog./isotope ratio mass spectrometry (GC/IRMS) method for stable C isotope anal. of amino acid enantiomers is presented. This method eliminates the numerous preparative steps integral to the isolation of amino acids and amino acid enantiomers from protein hydrolyzates that precede $\delta^{13}\text{C}$ anal. by conventional isotope ratio mass spectrometry. Unlike hydrocarbons, amino acids require derivatization prior to GC/IRMS anal. Replicate $\delta^{13}\text{C}$ analyses of trifluoroacetyl (TFA) iso-Pr ester derivs. of 22 amino acids by IRMS revealed that the derivatization process is reproducible, with an av. error (1 std. deviation) of $0.10\% \pm 0.09\%$. The av. anal. error for anal. of amino acid derivs. by GC/IRMS was $0.26\% \pm 0.09\%$. In general, abs. differences between IRMS and GC/IRMS analyses were $<0.5\%$. The derivatization process introduces a distinct, reproducible isotopic fractionation that is const. for each amino acid type. The obsd. fractionations preclude direct calcn. of underivatized amino acid $\delta^{13}\text{C}$ values from their resp. TFA iso-Pr ester $\delta^{13}\text{C}$ compns. through mass balance relation. Derivatization of amino acid stds. of known stable C isotope compn. in conjunction with natural samples, however, permits computation of the original, underivatized amino acid $\delta^{13}\text{C}$ values through use of an empirical correction for the C introduced during the derivatization process.

L14 ANSWER 67 OF 83 CA COPYRIGHT 2003 ACS

AN 81:55586 CA

TI Chemical information from computer-processed high resolution mass spectral data. Correction of intensities and conversion from isotopic species to equivalent chemical species

AU Hilmer, Richard M.; Taylor, James W.

CS Dep. Chem., Univ. Wisconsin, Madison, WI, USA

SO Analytical Chemistry (1974), 46(8), 1038-44

AB A significant decrease in the no. of possible formulas corresponding to peaks in a high-resoln. mass spectrum is achieved by converting the isotopic formulas to a single chem. equiv. formula. A weighting factor derived from the correlation of a given formula with the rest of the spectrum is used to delete all but the most significant formulas. For the test cases examd., the odd-electron species with the highest weighting factor usually corresponded to the correct mol. ion, when the mol. ion

intensity was greater than the **mass spectrometer** detection limits.

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STN INTERNATIONAL LOGOFF AT 10:24:44 ON 17 JUN 2003

=> d his

(FILE 'HOME' ENTERED AT 08:52:51 ON 17 JUN 2003)

FILE 'CA' ENTERED AT 08:53:01 ON 17 JUN 2003

L1 11349 S (MASS OR SPECIE) (1A) BALANCE
L2 18761 S CRIII OR CRIV OR (CR OR CHROMIUM) (W) (III OR IV)
L3 9 S L1 AND L2
L4 155 S L1 AND SPECIATION
L5 8 S L4 AND MASS SPEC?
L6 63 S L4 AND (TRACE OR REDOX OR REDUC? OR OXID? OR HYPHEN?)
L7 76 S L3, L5-6
L8 45 S L7 NOT PY>1998
L9 0 S L7 NOT L8 AND PATENT/DT
L10 50 S L4 NOT L5-6 NOT PY>1997
L11 94 S L8, L10

=> d l11 bib, ab 1-94

L11 ANSWER 5 OF 94 CA COPYRIGHT 2003 ACS

AN 129:264434 CA

TI **Speciation** of nickel emissions from oil-fired power plant

AU Bell, Arlene C.; Wong, John; Chu, Paul

CS Carnot, Tustin, CA, USA

SO Proceedings, Annual Meeting - Air & Waste Management Association (1996),
89th, tp5604/1-tp5604/14

AB The Elec. Power Research Institute (EPRI) in conjunction with host utilities sponsored a study to speciate nickel emissions at four oil-fired power plants. There was a need to characterize and det. the forms of nickel from oil-fired power plants because estns. of health risk by regulatory agencies may assume that 100% of nickel emissions from combustion sources are in the carcinogenic nickel subsulfide (Ni₃S₂) form; the limited data available has indicated that only a small fraction of nickel emitted from boilers is Ni₃S₂; and emissions of total nickel from uncontrolled oil-fired boilers are one to two orders of magnitude higher than from coal-fired boilers with particulate control. EPRI sponsored a program, conducted by Carnot and the University of Louisville Chem. Department, in which samples were collected and analyzed from four oil-fired boilers selected to achieve a range of boiler type, fuel sulfur level, NO_x control, and particulate control. The objectives of the program were: to det. the nickel species emitted from oil-fired utilities; to provide detailed nickel **speciation** data for use in health risk assessments; to provide detailed nickel **speciation** for use by individual utilities in permitting, inventory, and risk issues; and to construct a total nickel **mass balance** at each site through anal. of oil and available ash samples. This paper will present a description of the program design, the sampling and anal. techniques used, and a summary of preliminary program results.

L11 ANSWER 7 OF 94 CA COPYRIGHT 2003 ACS

AN 129:165764 CA

TI Problems in **trace** metal **speciation** modeling

AU Turner, David R.

CS Department of Analytical and Marine Chemistry, Goteborg University and

Chalmers University of Technology, Goteborg, 5-412 96, Swed.

- SO IUPAC Series on Analytical and Physical Chemistry of Environmental Systems (1995), 3 (Metal Speciation and Bioavailability in Aquatic Systems), 149-203
- AB A review with 126 refs. concerning problems in **trace metal speciation** modeling is given. Topics discussed include: chem. **speciation** in natural waters; natural water compn.; the equil. assumption; the **speciation** modeling process (concn. scales); complexation by dissolved inorg. ligands (modeling activity coeffs., major and minor elements [ion assocn. models of seawater, ion interaction models of seawater], **trace elements** [complications of stability consts., selection of activity coeff. models], summary and recommendations); complexation by small org. ligands; natural org. matter (nature and structure, standardized data descriptions [affinity spectrum, differential equil. function, mastercurve], models [non-electrostatic, electrostatic], summary and recommendations); adsorption (adsorption on **oxide** surfaces, ion exchange, adsorption onto natural particles, summary and recommendations); mixed ligand reactions (mixed ligand complexes in soln., mixed ligand adsorption reactions); **redox** reactions; and **speciation** modeling codes (theor. background [complexation and **mass balance** equations, **redox** reactions, adsorption (surface complexation) reactions, ion exchange], **speciation** codes).

L11 ANSWER 9 OF 94 CA COPYRIGHT 2003 ACS

AN 129:157746 CA

TI Method optimization and quality assurance in **speciation** analysis using high performance liquid chromatography with detection by inductively coupled plasma **mass spectrometry**

AU Larsen, Erik H.

CS Danish Veterinary and Food Administration, Institute of Food Chemistry and Nutrition, Soborg, DK-2860, Den.

SO Spectrochimica Acta, Part B: Atomic Spectroscopy (1998), 53B(2), 253-265

AB A review with 23 refs. Achievement of optimum selectivity, sensitivity and robustness in **speciation** anal. using high performance liq. chromatog. (HPLC) with inductively coupled **mass spectrometry** (ICP-MS) detection requires that each instrumental component is selected and optimized with a view to the ideal operating characteristics of the entire **hyphenated** system. An isocratic HPLC system, which employs an aq. mobile phase with org. buffer constituents, is well suited for introduction into the ICP-MS because of the stability of the detector response and high degree of analyte sensitivity attained. Anion and cation exchange HPLC systems, which meet these requirements, were used for the sepn. of selenium and arsenic species in crude exts. of biol. samples. Furthermore, the signal-to-noise ratios obtained for these incompletely ionized elements in the argon ICP were further enhanced by a factor of four by continuously introducing carbon as methanol via the mobile phase into the ICP. Sources of error in the HPLC system (column overload), in the sample introduction system (memory by org. solvents) and in the ICP-MS (spectroscopic interferences) and their prevention are also discussed. The optimized anion and cation exchange HPLC-ICP-MS systems were used for arsenic **speciation** in contaminated ground water and in an inhouse shrimp ref. sample. For the purpose of verification, HPLC coupled with tandem **mass spectrometry** with electrospray ionization was addnl. used for arsenic **speciation** in the shrimp sample. With this anal. technique the HPLC retention time in combination with mass anal. of the mol. ions and their collision-induced fragments provide almost conclusive evidence of the identity of the analyte species. The **speciation** methods are validated by establishing a **mass balance** of the analytes in each fraction of the extn. procedure, by recovery of spikes and by employing and comparing independent techniques. The urgent need for ref. materials certified for elemental species is

stressed.

L11 ANSWER 11 OF 94 CA COPYRIGHT 2003 ACS
AN 128:248194 CA
TI Modeling adsorption and desorption processes in estuaries
AU Turner, A.; Tyler, A. O.
CS Department of Environmental Sciences, University of Plymouth, Plymouth, PL4 8AA, UK
SO Cambridge Environmental Chemistry Series (1997), 9(Biogeochemistry of Intertidal Sediments), 42-58
AB An empirical method to study sorptive behavior of **trace** metals and **trace** org. compds. in estuaries is presented. The partitioning of constituents between particles and soln. is detd. exptl., without identifying the inherent reaction mechanisms or reactant **speciation**, under controlled lab. conditions using natural samples spiked with radiotracer analogs of the constituent of interest. Adsorption and desorption may be modeled as a function of particle concn., and the controlled variables, salinity and dissolved O concn., by incorporating empirically-derived results into simple **mass balance** equations. This approach is illustrated using site-specific results from two contrasting estuarine environments, the Clyde and Humber estuaries; calcd. results are discussed in the context of their agreement with field measurements of **trace** constituents in these estuaries.

L11 ANSWER 17 OF 94 CA COPYRIGHT 2003 ACS
AN 127:311147 CA
TI Aquatic colloids: concepts, definitions, and current challenges
AU Gustafsson, Orjan; Gschwend, Philip M.
CS R. M. Parsons Laboratory, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA
SO Limnology and Oceanography (1997), 42(3), 519-528
AB Colloidal phases in natural waters may be important to various environmental questions, esp. those concerning the cycling of vital and toxic **trace** chems. Current treatments of the role of colloids in chem. **speciation** largely rely on operational definition of phases such as 1000-dalton ultrafilter and 0.45- μ m filter cut-offs. Defining chem. phases exclusively by a phys. parameter such as size is contributing to a situation where the obsd. filterable vs. solute equil. consts. Achieving the goal of relating the natural distributions of chems. to theor. expectations is contingent upon progress in development of a functionally meaningful colloid definition and interpretation of obsd. distributions of **trace** substances in terms of the relevant physicochem. properties of the system. We assess the phase status of typical components in natural waters from a "chemcentric" point of view (i.e., one whose motivation is to understand the cycling of **trace** chems. in the environment). As a result, we define colloids so as to provide a thermodyn. grounding for evaluating chem. **speciation** and a hydrodynamic framework distinguishing phases that are transported with the soln. from those that are not. These constraints lead one to define an aquatic colloid as any constituent that provides a mol. milieu into and onto which chems. can escape from the aq. soln., and whose movement is not significantly affected by gravitational settling. Such a definition allows development of **mass balance** equations, suited to assessing chem. fates, that reflect processes uniquely acting on dissolved, colloidal, settling particle phases.

L11 ANSWER 20 OF 94 CA COPYRIGHT 2003 ACS
AN 127:224733 CA
TI Nickel **speciation** of fly ash by phase extraction
AU Wong, J. L.; Qian, J.; Chen, C. H.

CS Department of Chemistry, University of Louisville, Louisville, KY, 40292, USA
SO Analytica Chimica Acta (1997), 349(1-3), 121-129
AB Chem. **speciation** of Ni is necessary for risk assessment of fossil fuel fly ash. We used a std. coal fly ash in sequential extn. to show reproducibility and **mass balance** of Ni phase fractionation, and applied it to 2 field samples of oil fly ash. Nine distinct Ni phases were quantitated by voltammetry and characterized by cumulative extn. plots and dissoln. kinetics. They are further correlated with SEM/EDX anal. of the fly ash. This Ni **speciation** method reflects the difference in the combustion process in generating the 2 oil fly ash and allows comparison of their Ni distribution and bioavailability.

L11 ANSWER 22 OF 94 CA COPYRIGHT 2003 ACS
AN 127:99249 CA
TI Chemical **speciation** of chromium and nickel in the western Mediterranean
AU Achterberg, Eric P.; Van Den Berg, Constant M. G.
CS Department of Environmental Sciences, Plymouth University, Plymouth, PL4 8AA, UK
SO Deep-Sea Research, Part II: Topical Studies in Oceanography (1997), 44(3-4, EROS 2000 (European River Ocean System), The Western Mediterranean), 693-720
AB The chem. **speciation** of dissolved Cr and Ni was measured onboard ship in the western Mediterranean Sea using cathodic stripping voltammetry (CSV) during the winter of 1992 and summer of 1993. Vertical profiles for dissolved Cr(III) in the water column showed concns. 0-1.4nM, with highest concns. in the surface layer, possibly caused by photochem. conversion of Cr(VI) to Cr(III) during summer periods and by atm. inputs during winter periods. Enhanced Cr(III) levels also were encountered in the deeper Mediterranean waters and were attributed to mineralization of sinking biol. material and diffusion from sediments. Dissolved Cr(VI) concns. were 2-3nM, and total dissolved Cr concns. were 2-3.5nM. Lowest concns. of total Cr and Cr(VI) occurred in the surface Atlantic waters and highest levels in the deeper Mediterranean waters. Total dissolved Ni concns. were 1.5-5nM. Between 10 and 20% of the total dissolved Ni in the western Mediterranean appeared to be strongly organically complexed. Both labile and total dissolved Ni concns. were lower in the surface Atlantic waters than in the Mediterranean deeper waters. Little difference was obsd. between the data sets for winter and summer, indicating that the influence of seasonal changes on the **speciation** of Ni was small. A clear nutrient-like behavior was not apparent for Ni and Cr, and their vertical and horizontal distributions were mainly detd. by phys. processes. Dissolved budget results for Cr and Ni for the Valdivia and Discovery (data in parentheses) cruises of -572 (55) and -439 (369) tons/yr were calcd., indicating that the dissolved budgets for these elements were well balanced. The budget deficits and surpluses for dissolved Cr and Ni were small compared to the mass fluxes involved in the calcn. of the **mass balances**.

L11 ANSWER 28 OF 94 CA COPYRIGHT 2003 ACS
AN 126:123228 CA
TI A polarographic method of **speciation** for labile metal-ligand systems based on **mass-balance** equations. A differential pulse polarographic study at fixed ligand to metal ratio and varied pH
AU Cukrowski, Ignacy
CS Department of Chemistry, University of the Witwatersrand, Private Bag 3, WITS 2050, Johannesburg, S. Afr.
SO Analytica Chimica Acta (1996), 336(1-3), 23-36
AB A new equation for **speciation** of labile species by polarog. is derived. It

relates the obsd. shift in a peak potential and a decrease in a peak height with a change in the concn. of a free metal ion in a soln. The free metal ion concn. is controlled by the formation of complexes of the metal ion with ligands and is calcd. from **mass-balance** equations written for the metal-ligand system. This allows an incorporation into the ligand-metal system any no. of complexes, those which are known and those which are thought to be formed and for which formation consts. are calcd. As a test of this method, complexes of Cd(II) with the ligand N,N,N',N'-tetramethylethylenediamine are studied by differential pulse polarog. (DPP) at fixed ligand-to-metal ratio and varied pH. All known hydroxide species of Cd, including polynuclear species, were incorporated into the metal-ligand system. A good agreement was found between formation consts. calcd. in the present work from DPP and those reported previously from potentiometry. In addn., a new complex, viz. $\text{CdL}_2(\text{OH})^+$, was found and its formation const., as $\log \beta$, was estd. to be 8.94 ± 0.03 .

(L11)

ANSWER 38 OF 94 CA COPYRIGHT 2003 ACS

AN

123:292419 CA

TI

Main principles of direct and reverse geochemical modeling

AU

Gimeno, M. J.; Pena, J.

CS

Instituto de Tecnologia Nuclear, Centro de Investigaciones Energeticas, Madrid, 28040, Spain

SO

Estudios Geologicos (Madrid) (1994), 50(5-6), 359-67

LA

Spanish

AB

Geochem. modeling consists in the application of thermodyn. and physicochem. principles in the hydrogeochem. systems interpretation. Inverse modeling (**mass balance** calcns.), which uses obsd. chem. and isotopic data from waters and rocks to identify geochem. reactions responsible for them in a quant. way; and forward modeling, which attempts to predict water compns. and mass transfer that can result from hypothesized reactions, from obsd. initial conditions on water-rock system compns., were developed. Both of these models have intrinsic uses and limitations. For a system with adequate chem., isotopic, and mineralogic data, the inverse-modeling approach of **speciation** and **mass-balance** modeling provides the most direct means of detg. quant. geochem. reaction models. In contrast, for system with missing or inadequate data, reaction-path modeling provides an a priori method of predicting geochem. reactions. In some cases it is useful to combine forward modeling with the results from inverse models. The **mass-balance** results det. the net mass transfer along the flow path, but these results are only partially constrained by thermodyn. The forward modeling can be used both, to prove thermodyn. consistency for them, and to predict water quality at points where there are no enough data. Recent advances in geochem. modeling are focused on finding the most efficient numerical procedures for coupling geochem. reactions (both equil. and kinetic) with the hydrodynamic transport equations in compositionally-complex systems, on uncertainty anal., and on model validation for actual geochem. systems.

(L11)

ANSWER 42 OF 94 CA COPYRIGHT 2003 ACS

AN

123:40472 CA

TI

Interannual Variability in the **Speciation** and Mobility of Arsenic in a Dimictic Lake

AU

Splithoff, Henry M.; Mason, Robert P.; Hemond, Harold F.

CS

Ralph Parsons Laboratory, MIT, Cambridge, MA, 02139, USA

SO

Environmental Science and Technology (1995), 29(8), 2157-61

AB

A comparison of the **speciation** and concn. of As in the hypolimnion of the dimictic Upper Mystic Lake over 3 yr demonstrates the importance of **redox** conditions, and the role of sulfide, in controlling the fate and

distribution of As in aquatic systems. Hypolimnetic As concns. were typically less than 20 nM in the hypolimnion under low oxygen, but not sulfidic, conditions in the fall of 1991 and 1992, with >90% of the dissolved As as As(V). In 1993, however, an order of magnitude increase in concn. to 380 nM total As, and a change in **speciation** to 58% As(III), coincided with the appearance of sulfide in the hypolimnion in Oct. Equil. modeling and **mass balance** estns. suggest that Fe and As (as As(III)) were being released from the sediment during the heightened anoxia. During fall overturn, however, the concn. decreased in concert with the disappearance of sulfide and by Dec., As(V) was again the predominant species (77%; total As 61 nM). These results have important implications as wind-induced mixing in this lake can transport hypolimnetic waters to the surface, thereby enhancing the potential for drinking water and food chain contamination in this urban lake.

L11 ANSWER 43 OF 94 CA COPYRIGHT 2003 ACS

AN 123:40412 CA

TI Chromium in San Francisco Bay: superposition of geochemical processes causes complex spatial distributions of redox species

AU Abu-Saba, Khalil E.; Flegal, A. Russell

CS Department of Chemistry and Biochemistry, University of California, Santa Cruz, CA, 95064, USA

SO Marine Chemistry (1995), 49(2-3), 189-99

AB Processes controlling the geochem. cycle of Cr in San Francisco Bay were characterized with analyses of water samples from 25 stations distributed throughout the estuary. Mixing of water masses, localized inputs, in-situ redn., and sediment resuspension contributed to complex spatial distributions of dissolved ($<0.45 \mu\text{m}$) Cr(III) and Cr(VI), as well as suspended particulate Cr. Total dissolved Cr concns. in the bay were 1.9-8.3nM, with the max. concn. at the head of the estuary (the Delta) that was attributed to a relatively large input (5.2nM) of Cr(III) within the San Joaquin River. The calcd. Cr(III) scavenging residence time in that region was relatively long (>3 days) for a particle reactive trace metal, suggesting either localized inputs or complexation by colloidal/org. matter. There was also a relative excess (2.6nM) of Cr(VI) in another section of the Delta. **Mass balance** calcns. showed that excess was the same order of magnitude as reported point source loadings of Cr in that area. The subsequent depletion of Cr(VI), along with a concurrent increase in Cr(III) concn. in a shallow region of the Delta, was tentatively attributed to in-situ redn.

L11 ANSWER 59 OF 94 CA COPYRIGHT 2003 ACS

AN 118:37676 CA

TI Advanced quality control for zinc **speciation** investigations in human breast milk

AU Michalke, B.; Muench, D. C.; Schramel, P.

CS Inst. Oekol. Chem., Forschungszent. Umwelt und Gesundheit GmbH, Neuherberg, W-8042, Germany

SO Fresenius' Journal of Analytical Chemistry (1992), 344(7-8), 306-10

AB Information is provided about the reliability of results obtained in Zn-**speciation** analyses of human milk. For such analyses, convenient techniques (Michalke, B., et al., 1991), comprising **mass balances** of metal ligand, purity of analytes, etc., have been given. The influence of the liq. chromatog. eluent was evaluated. Twice-distd. water was compared with different buffers as the eluent. Water proved to be a more suitable mobile phase than buffers with regard to contamination. A method was developed to investigate the possibility of a transfer of Zn among the proteins during size exclusion chromatog. For these expts., casein and metallothionein

were chosen as competitive Zn ligands, showing extremely different affinities for Zn. A possible Zn transfer from one protein to the other was examd. in combining a Zn-contg. protein with a Zn-free one. No change of the Zn status of the proteins was detected, indicating a stable protein-metal complex under the exptl. conditions. Zn and protein **mass balances** (injected/eluted) were calcd. and found to be 100%.

L11 ANSWER 77 OF 94 CA COPYRIGHT 2003 ACS

AN 106:144941 CA

TI Calculation of equilibrium species for the aqueous solution systems of uranyl sulfate-uranium(IV) sulfate-sulfuric acid-hydrofluoric acid and uranyl chloride-uranium tetrachloride-hydrochloric acid-hydrofluoric acid at 298 K

AU Majima, Hiroshi; Awakura, Yasuhiro; Sato, Koji; Hirono, Shuichiro

CS Dep. Metall., Kyoto Univ., Kyoto, 606, Japan

SO Metallurgical Transactions B: Process Metallurgy (1987), 18B(1), 49-57

AB **Speciation** models for aq. solns. of UO_2SO_4 - $\text{U}(\text{SO}_4)_2$ - H_2SO_4 -HF and UO_2Cl_2 - UCl_4 -HCl-HF were proposed based on chem. reaction equil., **mass balances**, charge balance, and stoichiometry of $\text{UF}_4(\text{s})$. The equil. concns. of U and F- species in these solns. were calcd. at 298 K, and are of relevance to the electrolytic **redn.** of U(VI), followed by the pptn. of $\text{UF}_4(\text{s})$. The **redn.** ratios of U(VI) were set at 25, 50, 75, and 100%. In the sulfate system, the stable domains of U^{4+} , $\text{U}(\text{SO}_4)_4^{2-}$, UF_4 -nn, and $\text{UF}_4(\text{s})$ as U(IV) species and UO_2^{2+} , $\text{UO}_2(\text{SO}_4)_2^{2-}$, and UO_2F_2 -nn, as U(VI) species are strongly dependent on the $\text{CT}(\text{F})/\text{CT}(\text{U(IV)})$ value. The stable domains of U^{4+} , UCl_3^+ , UF_4 -nn, and $\text{UF}_4(\text{s})$ as U(IV) species and UO_2^{2+} , UO_2Cl^+ , and UO_2F_2 -nn as U(VI) species are also strongly affected by the $\text{CT}(\text{F})/\text{CT}(\text{U(IV)})$ ratio in the chloride system. The initiation and pptn. of $\text{UF}_4(\text{s})$ in both the sulfate and chloride systems are functions of the **redn.** ratio of U(VI). The higher the **redn.** ratio, the lower the $\text{CT}(\text{F})/\text{CT}(\text{U(IV)})$ values required. Compared to the chloride system, $\text{UF}_4(\text{s})$ pptn. in the sulfate system starts at a lower value of $\text{CT}(\text{F})/\text{CT}(\text{U(IV)})$. The addn. of an excess amt. of HF does not cause the dissoln. of $\text{UF}_4(\text{s})$ ppts. because HF is a weak acid.

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AN 91:9242 CA

TI WATEQ2 - a computerized chemical model for **trace** major element **speciation** and mineral equilibria of natural waters

AU Ball, James W.; Jenne, Everett A.; Nordstrom, Darrell Kirk

CS Water Resour. Div., U. S. Geol. Surv., Menlo Park, CA, 94025, USA

SO ACS Symposium Series (1979), 93(Chem. Model. Aqueous Syst.: Speciation, Sorption, Solubility, Kinet.), 815-35

AB The computerized aq. chem. model of A. H. Truesdell and B. F. Jones (1973, 1974) as been revised and expanded to include ion assocn.- and soly. equil. for Ag, As, Cd, Cu, Mn, Ni, Pb, and Zn, soly. equil. for various metastable and/or sparingly sol. equil. solids, calcn. of propagated std. deviation, calcn. of **redox** potentials from various couples, polysulfides, and a **mass balance** section for sulfide solutes.

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AN 86:145297 CA

TI Analysis for chromium traces in the aquatic ecosystem. II. A study of **chromium(III)** and chromium(VI) in the Susquehanna River Basin of New York and Pennsylvania

AU Pankow, James F.; Leta, Daniel P.; Lin, Joyce W.; Ohl, Steven E.; Shum, Wilfred P.; Janauer, Gilbert E.

CS Dep. Chem., State Univ. New York, Binghamton, NY, USA

SO Stevens Report, Stevens Institute of Technology (1977), 7(1), 17-26

AB The persistence of Cr(VI) at least as far as 60 km downstream of the outfall led to the conclusion that, at the levels noted, little dissolved Cr(VI) is removed from the river as it flows away from the outfall. Cr concns. in river sediments also revealed Cr contamination below the outfall area, and Cr contamination extended at least as far as 60 km downstream from the outfall. A procedure was developed for the differential anal. of the ppb concns. of **Cr(III)** and **Cr(IV)** in natural waters; 3-L samples are filtered, acidified to pH 6.0, and divided. Then, 1 L is passed through an anion-exchange resin bed (AG-1X4, 100-200 mesh, Cl⁻ form), 1 L is passed through a cation-exchange resin bed (50 WX4, 100-200 mesh, Na⁺ form), and 1 L remains untreated. Each aliquot then receives 10 mL of 1.0M HNO₃ and each is then reduced in vol. to 10 mg. Anal. by at. absorption employing the method of std. addn. follows. By difference, cationic, anionic, and nonionic Cr concns. are detd. **Cr(III)** concn. was probably closely related to cationic and nonionic and Cr(VI) concn. in the original sample corresponded to the anionic portion. Precision was $\pm 20\%$ or above for total, cationic, and anionic Cr at the 1 ppb level. The precision of the nonionic anal. was closely linked to these other precisions as the concn. of nonionic Cr species in the original sample was obtained by the **mass balance** requirement set up by the other 3 analyses. Application of the technique to the anal. of natural water samples revealed the predominance of Cr³⁺ in uncontaminated waters of the Upper Susquehanna River Basin (1-2 ppb). River water samples taken downstream of the Binghamton, N.Y., area sewage outfalls revealed an increase of the mean Cr(VI) concn. in the river from 0.5 to 1.6 ppb.

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